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This is the end of the first year of an AFOSR-sponsored program to investigate the mechanisms of cyclic and monotonic deformation in Ni₃Al and NiAl as a function of loading mode (uniaxial vs. multiaxial) temperature, strain rate and environment. The program has analytical, numerical, and experimental aspects. The premise of the program is that it is important to understand these phenomena if ordered alloys are to be used in advanced jet engine components with some degree of confidence.

In the period just completed, significant theoretical contributions towards understanding deformation in Ni₃Al as a function of temperature and strain rate have been made. Starting with fundamental thermodynamics and dislocation mechanics, it has been demonstrated for the first time that the

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Georgia Tech

June 14, 1991

Dr. Alan Rosenstein
Deputy Director for Electronic and Material Sciences
Air Force Office of Scientific Research
Bolling AFB, Building 410
Washington D.C., 20332

Dear Dr. Rosenstein:

Enclosed are 6 copies of a progress report on grant # AFOSR-90-0162 entitled **"Deformation, Constitutive Behavior and Damage of Advanced Structural Materials Under Multiaxial Loading"** for the period 06/01/90 - 05/31/91. We believe that we are making excellent progress, especially in the area of theoretical modelling of deformation processes in ordered materials.

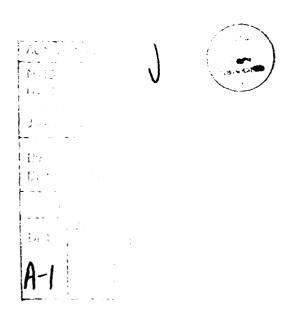I am looking forward to hearing from you and to any comments that you may have.

Sincerely,

Stephen D. Antolovich
Professor and Director
School of Materials Engineering
Director, Mechanical Properties Research Laboratory

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DEFORMATION, CONSTITUTIVE BEHAVIOR AND DAMAGE
OF
ADVANCED STRUCTURAL MATERIALS UNDER MULTIAXIAL LOADING

PREPARED BY:

Stephen D. Antolovich   6/14/91

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Technical Report

Progress Report for period 06/01/90 through 05/31/91
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Air Force Office of Scientific Research
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Program Manager: Dr. A.H. Rosenstein

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I. PROGRAM OVERVIEW

This is the end of the first year of an AFOSR-sponsored program to investigate the mechanisms of cyclic and monotonic deformation in Ni_3Al and NiAl as a function of loading mode (uniaxial vs. multiaxial) temperature, strain rate and environment. The program has analytical, numerical, and experimental aspects. The premise of the program is that it is important to understand these phenomena if ordered alloys are to be used in advanced jet engine components with some degree of confidence.

In the period just completed, we have made what we believe are major theoretical contributions towards understanding deformation in Ni_3Al. We have also made an extensive review of the literature of NiAl type ordered alloys and are in position to begin some multiaxial experiments on NiAl.

II. INTRODUCTION

Ordered intermetallic alloys possessing long range atomic order and forming superlattice structures are being extensively studied for high temperature applications which are currently dominated by superalloys. These alloys generally exhibit excellent resistance to corrosion and oxidation at elevated temperatures. The long range order causes slower diffusion rates and thus improves creep resistance. In these structures, dislocation motion depends on various factors which either enhance or inhibit dislocation mobility depending upon temperature [1-7]. The strength of these materials does not decrease drastically with temperature as seen in other disordered alloys, and in some cases the yield stress actually increases with temperature. Inspite of all the desirable properties possessed by these materials, inherent brittleness has severely limited their applications. This brittleness is due to weak grain boundaries for NiAl and Ni_3Al and limited number of permissible slip systems for NiAl. Among the various materials studied, most attention has been focussed on studying the mechanical behavior of intermetallics like Ni_3Al and NiAl. While a significant amount

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of data is available on the deformation characteristics of single and polycrystalline Ni_3Al under various loading and environmental conditions, a complete understanding of the deformation characteristics of NiAl is yet to be achieved. The purpose of this study is to investigate deformation behaviour of Ni_3Al and NiAl under different loading conditions (uniaxial, multiaxial, monotonic and cyclic) and temperatures.

Ni_3Al which possesses the $L1_2$ structure exhibits extreme ductility in single crystal form and is equally brittle in polycrystalline form [8]. The fracture surface revealed intergranular fracture mode implying that weak grain boundaries formed the fracture path [9]. Additions of alloying elements like B and Cr have eased the problem of grain boundary weakness, resulting in significant increases in ductility, yet it remains to be seen how these additions behave in different environments [10-14]. At this point it is necessary to investigate the creep and fatigue response of these alloys under different environmental and thermal conditions before using them for any structural use.

Another intermetallic in the Ni-Al system having a B2 structure and possessing excellent properties (i.e high melting point (1950 K), high isothermal and cyclic oxidation resistance and density about 30% less than conventional superalloys), is NiAl. Negligible room and low temperature ductility, and rapid loss of strength with temperature have prevented the use of these materials as possible replacement to conventional superalloys. The mechanical behavior of NiAl has been studied by various researchers [15-19] but the fundamental deformation mechanisms have not been fully understood. Efforts to improve room temperature ductility range from microalloying techniques to generating interfacial dislocation sources in an effort to satisfy the von Mises criterion for generalized plastic deformation.

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III. DEFORMATION CHARACTERISTICS OF Ni₃Al

A. DISLOCATIONS IN Ni₃Al

The principal operating slip system in Ni_3Al is $\{111\}<010>$. Since the length of the unit dislocation in a superlattice is twice that of the unit dislocation in a FCC lattice it is energetically favorable for a superdislocation to dissociate into a pair of superpartials separated by a strip of antiphase boundary (APB). As a result, under the influence of the various constraints imposed by the long range order of the superalttice several different combinations and faults[20] have been observed in these materials.

Computer simulation studies have shown that the dislocations in $L1_2$[21,22] type of materials have non-planar core configurations and so the components of the shear stress which do not exert a resolved shear stress on the dislocation can drastically change the overall deformation charactersitics of Ni_3Al by altering the core dissociations[3-5].

B. DEFORMATION IN Ni₃Al

Ni_3Al and several other $L1_2$ materials, in both, single crystal and polycrystalline form exhibit two different deformation regimes as function of temperature [3,4,6,8,23]. The initial regime is characterized by a steady increase in flow stress with temperature up to a peak value ranging from 850-1250 K. Deformation in this regime occurs by the operation of the $\{111\}<110>$ slip (primary octahedral slip). Some of the other unusual deformation characteristics in this regime include:

1. Schmid law failure [3]

2. Orientation dependent tension-compression asymmetry [4]

3. Strain rate independence [2,3,23]

4. Thermal reversibility. [8,14]

In the second regime, a continuous decrease in strength with temperature is seen. $\{010\}<110>$ slip (primary cube slip) is the primary slip system [2-4,6,8,23]. Diffusion

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assisted dislocation motion, lower density of dislocation barriers, and higher Schmid factor are the reasons for which cube slip is preferred over octahedral slip. These two regimes are separated by a peak where the principal operating slip system changes from primary octahedral to primary cube. The value of the peak depends on the orientation.

Various models have been proposed to describe the deformation behavior of these materials. The ones currently accepted are:

1. Partial cross-slip (Cross-Slip Pinning (CSP)) model [5,24-27]

2. Total cross-slip model. [1,28,29]

Each of the above theories will be discussed briefly.

1. Cross-Slip Pinning Model

This model based on the foundations laid by the initial work of Takeuchi and Kuromuto[3], Lall et al[4] and the computer simulation studies of the core structure of the dislocations[21,22], attributes the anomalous yielding to a thermally activated cross slip of small segments of the superdislocation from {111} to {010} planes. This mechanism is then believed to produce a sessile-glissile configuration where the sessile cross-slipped segments prevent further glide of dislocations lying on {111} planes. This increases the stress necessary to cause further deformation. Based on thermodynamic arguments, the density of cross-slipped segments increases with temperature resulting in increasing yield stress with temperature.

2. Total Cross-Slip Model

Opposing the above model based on its apparent inability to explain the strain rate independence of the yield stress[1], is the model proposed by Sun and Hazzeldine[28]. This

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[1]As discussed later, we have proposed a modification of the Cross-Slip Pinning model which is capable of explaining all of the important deformation-related observations, including the apparent strain rate insensitivity.

model is based on the weak beam observations of deformed $L1_2$ alloys which showed the APB of Kear-Wilsdorf locks to lie entirely on the cube plane[28,30,31,32]. The concept of diffusion assisted motion of dislocations first visualized by Flinn[1] forms an integral part of the theory which describes the deformation response of $L1_2$ intermetallics as being governed by the motion of kinks on the primary octahedral plane.

Recently, de Bussac *et al* [33,34] presented the results of studies to understand the time dependency of the cross-slip kinetics. It was proposed that cross-slipping in $L1_2$ alloys is an instantaneous process and a thermodynamic approach was used to explain the various aspects of deformation mechanism. Chapter 4 describes the analytical and experimental considerations of the above model.

Polycrystalline Ni_3Al, in contrast to single crystals, exhibits extreme brittleness. SEM studies of the fracture surface reveal a intergranular fracture morphology implying that the inherent brittleness of polycrystalline Ni_3Al is largely due to weak grain boundaries. It has been demonstrated that room temperature ductility of Ni_3Al can be increased by microalloying Ni_3Al with small amounts of B[10]. Webb and Antolovich[14] and Matuszyk *et al*[35] have further studied the effects of environment on the mechanical behavior of B and Cr doped Ni_3Al at ambient and elevated temperatures. It was observed that Ni_3Al failed by brittle fracture at elevated temperatures in air. The presence of oxygen at grain boundaries was considered as the primary reason for low high temperature ductility. Techniques to overcome environmental embrittlement involve eliminating grain boundaries oriented perpendicular to the stress axis [36] and strategic alloying [13]. Small additions of Cr promote oxide formation at the grain boundaries which reduces the concentration of atomic oxygen at grain boundaries[13]. The effect of B has been argued to either promote mobility of grain boundary dislocations or to increase the intrinsic grain boundary strength. Based on the most recent evidence, the grain boundary strengthening appears most logical[37].

Although it is evident from the discussion so far that Ni_3Al can be used as a structural material for high temperature applications, further knowledge regarding its mechanical behavior under multiaxial loading conditions is essential. A knowledge of the complex stress distribution pattern prevailing during multiaxial loading would provide additional insights to the present understanding and also help in directing further research towards the development of two phase alloys for high temperature, high stress applications.

C. CHARACTERSITICS OF CYCLIC DEFORMATION.

Experiments to study the cyclic deformation of single crystal $L1_2$ alloys indicate that the orientation dependent tension-compression asymmetry observed in Ni_3Al subjected to normal loading conditions, is stable during cyclic loading [38-41] below the peak strength. The increase in stress due to cyclic hardening was found to depend on temperature, crystallographic orientation, and applied strain range [38-40]. Such observations were also made in PWA 1480 which has about 65% γ'[42].

TEM observations of the deformed specimen revealed long, straight screw dislocations [14,39,43] and dislocation debris due to dislocation interactions. The distribution of dislocations within the slip bands was inhomogeneous which led to localized stress concentrations and finally fracture. Intersecting mobile dislocations left behind screw and edge dipoles [43]. It was also claimed that Frank loops were observed by Hsuing and Stoloff[39]. However this observation has never been replicated and may have been an artefact of TEM. TEM observations of the studies conducted by Webb *et al* [14] revealed the presence of APB coupled screw dislocations, mixed, edge, and screw dipoles and SISF faults associated with dislocations. These dislocations were homogeneously distributed throughout all grains predominantly on the primary $\{111\}<010>$ slip system. Studies to investigate the cyclic response of Ni_3Al revealed that the strength in compression was always greater than in tension[42]. This stress asymmetry was due to reversibility of slip where the

pinning points in tension become unpinned during stress reversal and may become pinned during compression at a different rate. Environmental changes affected the fatigue life, even though cyclic hardening to saturation was independent of environment. When tested in air, fracture occurred prior to saturation while the specimen tested in vacuum had a fatigue life two orders of magnitude higher than the one tested in air. Increasing the strain rate by an order of magnitude doubled the fatigue life for a given strain range.

The differences in dislocation interactions and the morphologies of the specimen deformed in air and in vacuum were clearly evident from TEM observations. It was observed that the proportion of dislocation debris in vacuum tested specimen was much higher than the one tested in air. This indicates that in the absence of oxygen, the material can withstand much larger amounts of dislocation debris before failure. The increase in fatigue life in vacuum was due to the absence of oxygen, whereas environmental conditions controlled fatigue in air.

Studies of crack propagation rates in Ni_3Al indicated a strong temperature dependence[14,32,43-45]. The crack growth rates increased with increasing temperature. Besides temperature, environment and frequency of loading also affected the growth rates. Additions of Cr increased the fatigue crack growth resistance in air at elevated temperature. The fracture morphology changed from intergranular at ambient temperatures to transgranular at high temperatures for specimens tested in air and showed a transgranular pattern for all specimens tested in vacuum.

IV. DEFORMATION CHARACTERISTICS OF NiAl

A. DISLOCATIONS IN NiAl

Dislocations in NiAl observed under TEM indicate a strong orientation dependence. Crystals oriented along [001] (hard orientation) deform by a slip vector $b = a_o <111>$ whereas all non-[001] crystals (soft orientation) have a slip vector $b = a_o <001>$ [46]. $<111>$ slip is

observed for <001> orientations because the resolved shear stress on any plane containing the <001> direction is near zero for such orientations and the stress required to deform is several times higher than that for other orientations. Slip in B2 materials is strongly influenced by the ordering energy which is very high in the case of NiAl. Although slip occurs on densely packed planes as observed in BCC, the slip direction is not necessarily the same. The ordering energy dictates the nearest neighbor distances for the involved atoms. Several studies have been conducted to predict the active slip systems in NiAl on the basis of ordering energy and anisotropic elasticity theory. On the basis of ordering energy Rachinger and Cottrell[47] predicted <001>{110} slip for energies greater than 0.06eV/atomic bond. On the other hand Ball and Smallman [15,48] assumed the ordering energy to be proportional to $KT_c/4$ and calculated the critical ordering energy to be 0.04eV/atomic bond which implied <111>{110} slip. However, actual calculations based on dislocation energies and mobilities predicted <001>{011} to be the operative slip system. This prediction was also made by Potter[49] using anisotropic elasticity theory for dislocations and ordering energy. It was later confirmed by TEM investigations of NiAl[48,49]. Cube slip (*i.e.* <100>{100} slip) which is predicted to occur at slightly higher stresses than for <001>{110} slip have been also been observed [17,48,49] in <110>-oriented single crystals.

TEM studies on deformed NiAl revealed that APB does not exist in NiAl [15,48,49] and so the mechanism of a superdislocation dissociating into a pair of superpartials does not occur NiAl. In the B2 lattice an a_o<001> Burgers vector was confirmed to be the operative slip vector by Pascoe and Newey [16] using surface slip trace analysis and by Loretto and Wasielewski [17] from TEM observations of deformed [112] oriented single crystals. Slip systems operative in soft orientation (*i.e.* non-[001] orientation) single crystals are also believed to operate in polycrystalline NiAl.

For hard orientation single crystals, several deformation mechanisms are observed

over a wide range of temperatures. A complete list of slip systems operating at different temperatures is presented in ref [46]. Briefly, <111> slip was observed in [001] single crystals at 77K [15,50,51]. Kinking and deformation by uniform slip was observed at temperatures ranging from 300-700K [50-53]. At temperatures greater than 700K climb and glide of a_o<111>, a_o<011>, and a_o<001> was observed [15,50-53].

B. CHARACTERISTICS OF MONOTONIC DEFORMATION IN NiAl

Deformation in NiAl is highly anisotropic. NiAl is extremely brittle in tension but exhibits significant ductility (>50% plastic strain) in <011> single crystals tested in compression [15]. However this does not imply that NiAl is ductile at room temperature. It is also wrong to assume that NiAl exhibits ductility in compression. Crystals oriented along the [001] direction failed to exhibit the ductility observed in <011> oriented crystals. Orientation, loading direction, and material quality seem to affect compressive ductility.

Darolia *et al* [54] failed to observe any room temperature tensile ductility in <001> single crystals. Tensile ductility of about 2% was observed in fine grained polycrystalline NiAl at room temperature [18,55]. The general consensus from the results of various studies presented above is that the operative slip system in NiAl is <001>{110} and possibly <001>{100} for soft orientations. It is clear that there are only three independent slip systems which are mutually perpendicular and do not satisfy the von Mises criteria [56-57] for plastic deformation which requires the operation of five independent slip systems. <111> slip observed in single crystals oriented along [001], could provide the additional slip systems but fracture occurs prior to yielding in hard orientation single crystals [18], which means that the flow stress in Ni Al for <111> slip is at least higher than the fracture stress.

Attempts have been made to improve room temperature ductility and high temperature strength of these alloys by introducing a second phase [46], addition of alloying elements, refining the grain size, and surface film softening. It is believed that the lack of

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ductility due to non-availability of five independent slip systems can be overcome by generating geometrical dislocations necessary for accommodating large plastic strains [58]. Stress concentrators, such as microcracks, grain and interphase boundaries, and surface films can act as dislocation sources.

1. Grain Boundary Dislocation Sources

Grain boundaries can generate dislocations and contribute to plasticity of a material. Dislocations present in the grain boundaries serve as dislocation sources. The density of grain boundary dislocation sources controls the density of generated dislocations. Thus a fine grained material having larger grain boundary area would generate more dislocations than a larger grain sized material than a fine grain sized material is expected to exhibit more plasticity than a coarse grained material.

2. Interphase Boundary Dislocation Sources

An interphase boundary separates two phases having different elastic, plastic, and physical properties. Depending upon the degree of mismatch of the lattice types of the two phases, the interphase boundary could be coherent, semi-coherent or coherent. When the boundary is not coherent, incoherency strains due to lattice mismatch which develop at the boundary can be relieved by the presence of misfit dislocations. These misfit dislocations generate dislocations in the matrix [58,59] and may contribute to the plasticity of the otherwise brittle matrix. Due to the differences in mechanical properties of the two phases, it is possible that one phase would deform more readily than the other. The deformation gradient which exists at the interphase region results in the generation of dislocations as suggested by Ashby's model [57] which may control the overall plasticity of the alloy.

Noebe et al[46] studied the role of surface and interfacial dislocation sources in a NiAl-based composite containing Ni_3Al (γ') as the second phase. Tensile elongations of about 8% at 300 K were obtained in an $Ni_{70}Al_{30}$ in-situ composite consisting of 40% β phase.

But a $<001>$ $Ni_{60}Al_{40}$ single crystal failed by brittle fracture prior to yielding. Microscopic examination revealed that the γ' fibers which showed considerable necking served as the ductile reinforcing phase. The matrix which is mainly the β phase failed by cleavage. TEM studies revealed that the entire interphase area served as a dislocation source. $a_o<001>$ and $a_o<011>$ dislocations were observed in the β and γ' phases respectively.

C. CHARACTERISTICS OF CYCLIC DEFORMATION

The presence of long range order leads to differences in the cyclic response of ordered and disordered alloys. Stoloff et al[45] studied the influence of long range order on the fatigue response of intermetallics which could be disordered by heat treatment and confirmed that long range order enhances high cycle fatigue resistance. The effects of environment, temperature and stoichiometry were also studied. The presence of oxygen and hydrogen were found to reduce the resistance to fatigue at high and low temperatures respectively. H. Wunsch and R. Gibala [60] studied the cyclic deformation of B2 aluminidies. Two alloys, $Fe_{60}Al_{40}$ and $Ni_{50}Al_{30}Fe_{20}$, prepared by rapidly solidified powder extrusion at different temperatures were tested under total strain control. A lower extrusion temperature resulted in increased accumulation of plastic strain for $Ni_{50}Al_{30}Fe_{20}$ alloy similar to what was observed in NiAl by Vedula et al [55]. A large stress asymmetry was observed only for the $Fe_{60}Al_{40}$ alloy. They also studied the effect of surface film softening on the ductility enhancement for cyclically deformed alloys. TEM analysis showed an inhomogenoeus dislocation substructure where some grains deformed more than others and slip was confined to well defined bands. While studies have been conducted to study the cyclic deformation behavior of B2 structures there are more questions than answers. Further work is necessary to understand the cyclic response under various environmental and thermal conditions. Investigations of the effects of long range order, strain amplitude, and relationships between crack initiation, superlattice dislocations, persistent slip bands are necessary. A thorough knowledge of all the aspects of

cyclic, monotonic and multiaxial deformation is a must before NiAl can be used to replace conventional superalloys.

V. A NEW MODEL FOR YIELDING IN Ni₃Al

A. THEORETICAL DEVELOPMENTS

In this section, recent developments for analytically describing deformation in ordered $L1_2$ alloys will be reported.

Previous descriptions for thermal strengthening in Ni_3Al (and like $L1_2$ ordered alloys) [3-5,24-27], have modelled deformation in the form of a kinetic process. These models have, in one form or another, provided expressions for the activation barrier associated with the forward cross-slip of small segments of glissile screw dislocations onto a planes where they are sessile. The inherent time dependency associated with such kinetic descriptions have resulted in inconsistencies with the observed strain rate independence of yield strength. Recent calculations for the kinetics of cross-slip [34], have demonstrated that the accumulation of cross-slipped segments in Ni_3Al is virtually instantaneous. These predictions were then employed to demonstrate that deformation is independent of the applied strain rate. Following in the vein of these calculations, a new model was proposed based upon the postulate that deformation in Ni_3Al is better described in terms of thermodynamic equilibrium [33]. These new concepts were also used to critically examine the commonly accepted dynamical break away mechanism for thermal strengthening. This mechanism was found to be inconsistent with the concepts of strain rate independence and thermodynamic equilibrium, and as such, a new mechanism was proposed and subsequently modelled.

The new mechanism asserted that a thermodynamically predictable number of small

cross-slip segments are always present on the screw dislocation line during deformation. These segments are presumed to exert a uniform drag stress which causes the dislocation to remain straight while gliding. Since both forward and reverse cross-slip of the pinning points are allowed in the mechanism, the location of the pinning points changes from one instant of time to another. However, the number pinning points remains constant. From this mechanism, calculation of the free-energy changes experienced from the initial to equilibrium state were made and used to derive a model for predicting the yield strength of Ni_3Al. In this initial analysis, entropy effects were ignored as they were presumed to be small. The derivation yielded an expression which could be used to predict all deformation characteristics of Ni_3Al, but required a positive driving force in order to predict thermal strengthening. The initial form of the thermodynamic model was criticized for this requirement which, although allowable, was not conceptually appealing. Recently, a refined analysis has been conducted in which the effects of entropy are included. This has resulted in a more appropriate expression for describing deformation of Ni_3Al in terms of thermodynamic equilibrium, which is not only consistent with all known deformation characteristics, but also eliminates the need for a positive driving force.

B. Model Assumptions

Assume a Ll_2 material which hardens as temperature increases. Thermal strengthening is derived from a distribution of p cross-slipped segments along the dislocation. The size of these segments is small ($l = n \cdot b$) compared to the total line length of dislocation ($L = N \cdot n \cdot b$). The cross-slipped segments impart a drag force per unit length which forces the dislocation to remain straight while gliding. Here n is the number of

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Burgers vectors in a cross slipped segment and N is the number of segments.

C. Calculation of System Entropy

The configurational free energy change associated with the distribution of pinning points is given exactly by:

$$\Delta S_{sys} = k \cdot \ln W \qquad (1)$$

where
W = number of possible configurations
k = Boltzman's constant

From elementary statistics, W can be approximated as:

$$W = N!/p! \cdot (N-p)! \qquad (2)$$

substituting (2) into (1) and using Sterling's approximation ($\ln X! = X \cdot \ln X - X$) gives:

$$\Delta S_{sys} = k \cdot [N \cdot \ln N - p \cdot \ln p - (N-p) \cdot \ln(N-p)] \qquad (3)$$

dividing through by N gives,

$$\Delta S_{sys}/N = k \cdot [\ln(N/N-p) - p/N \cdot \ln(p/N-p)] \qquad (4)$$

D. Calculation of the System Free Energy Change

Given the enthalpy change associated with the formation of a single cross-slip segment of length $n \cdot b$, ΔH, (for which several expressions have been provided [5,24-27]) the free energy change of the <u>system</u> of p cross-slipped segments can be expressed as:

$$\Delta G_{sys} = p \cdot \Delta H - T \Delta S_{sys} \qquad (5)$$

or on the basis of a single segment:

$$\Delta G_{sys}/N = p/N \cdot \Delta H - T \cdot \Delta S_{sys}/N \qquad (6)$$

Defining the *concentration* of cross-slipped segments X by:

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$$X = p/N \tag{7}$$

inserting equation (4) into (6) and substituting (7) yields:

$$\Delta G_{sys}/N = X \cdot \Delta H - k \cdot T \cdot [\ln(1/(1-X) - X \cdot \ln(X/1-X)] \tag{8}$$

At equilibrium, the system free energy is minimized. The concentration of cross-slipped segments which occurs at equilibrium X_{eq} can be determined by:

$$\tag{9}$$

$$\frac{\partial G_{sys}/N}{\partial X} = 0$$

differentiation of equation (8) with respect to X yields:

$$\Delta H = k \cdot T \cdot \ln[1\text{-}X/X] \tag{10}$$

which can be rearranged to yield:

$$X_{eq} = 1/[1 + \exp(\Delta H/k \cdot T)] \tag{11}$$

Equation (11) describes the equilibrium concentration of cross-slipped segments in terms of the enthalpy of formation of a single pinning point.

E. An Equilibrium Model for Thermal Strengthening

Recalling the mechanism for thermal strengthening by a thermodynamic concentration of small pinning points X_{eq}, the yield strength of such materials can be expressed as [33]

$$\tau_{ys} = \tau_o \cdot X_{eq} \tag{12}$$

Substitution of equation (11) into (12) provides an expression for the yield strength at thermodynamic equilibrium.

$$\tau_{ys} = \tau_o/[1 + \exp(\Delta H/k\cdot T)] \qquad (13)$$

At large values of ΔH, $\Delta H/k\cdot T >> 1$ and

$$\tau_{ys} = \tau_o\cdot\exp(-\Delta H/k\cdot T) \qquad (14)$$

Equations (13) and (14) provide theoretical basis for thermal strengthening due to the creation of small cross-slipped segments along the dislocation line provided the system is at equilibrium, and ΔH is positive (i.e. ignoring volume effects the energy of the system with the cross-slipped segments is higher than without them). Previous work [34] has demonstrated that provided the size of such segments is relatively small (i.e. n < 3), equilibrium is achieved quasi-instantaneously ($t_{ch} \approx 10^{-8}$ sec).

Utilization of equation (14) provides theoretical basis for description of the observed deformation properties of Ni_3Al and like Ll_2 alloys. These include strain rate independence and thermal reversibility, in addition to thermal strengthening, Schmid factor violation, and tension-compression asymmetry. Several forms of stress-modified activation enthalpy have been proposed [5,24-27] which are suitable for insertion into equation (14). As these analytical descriptions are fairly well known, they will not be addressed here.

VI. Interactions and Reporting

Good relationships exist with C.T. Liu (ORNL) and Erland Schulson (Dartmouth College). In addition a good working relationship has been established with Dr. Randy Bowman of NASA-Lewis Research Center. Dr. Bowman worked on a previous AFOSR grant and is now considered to be one of the leading authorities on TEM in ordered compounds. He acts as an unpaid consultant and as a coordinator with NASA projects in this area.

We expect to be publishing a number of articles in the up-coming year on advances that we have made in theoretical modelling. The paper is authored by Graham Webb, Stephen D. Antolovich, and Arnaud de Bussac. We also anticipate having sufficient information on multiaxial deformation of NiAl and Ni$_3$Al to have a publication ready for submission towards the beginning of 1992.

VII. Personnel

Mr. Graham Webb is a Graduate Research Assistant supported by this project and working towards his Ph.D. His major contributions have been in the area of theoretical modelling. He will complete his Ph.D. in August, 1991.

Mr. Ritesh Shah is a Graduate Research Assistant who started on his Ph.D. program in Jan. 1991. He is responsible for mechanical testing and for computer modelling of deformation processes.

Mr. Rick Brown is a Research Equipment Specialist in the Mechanical Properties Research Laboratory at Georgia Tech and is involved with experimental set-ups and with assisting and training students.

In addition to the above personnel, clerical assistance has been provided by Ms. Janice Coleman. Administrative and financial assistance is provided by Ms. Pat Ledon and by Ms. Robin Green, all of the School of Materials Engineering.

VIII. Plans for the Next Year

During the next project period we intend to concentrate on multiaxial deformation of NiAl using currently available materials. We also anticipate that there will be some Ni$_3$Al available from a previous AFOSR program that will allow us to carry out some multiaxial

studies of this material as well. We have also received permission from NASA-Lewis Research Center to use their facilities for making single crystals of NiAl which can be used to further our fundamental deformation studies. We plan to fabricate the single crystals in the late Summer and hope to have specimens available for testing by late Fall, 1991.

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